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Combining Petroleum Coke and Natural Gas for Efficient Liquid Fuels Production

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ABSTRACT

This work explores the technical feasibility and economic profitability of converting petroleum coke (petcoke) and natural gas to liquid fuels via Fischer-Tropsch synthesis. Different petcoke conversion strategies were examined to determine the conversion pathway which can be competitive with current market prices with little or no adverse environmental impacts. Three main design approaches were considered: petcoke gasification only, combined petcoke gasification and natural gas reforming through traditional processing steps, and combined petcoke gasification and natural gas reforming by directly integrating the gasifier's radiant cooler with the gas reformer. The designs investigated included scenarios with and without carbon capture and sequestration, and with and without CO₂ emission tax penalties. The performance metrics considered included net present value, life cycle greenhouse gas emissions, and the cost of CO₂ avoided. The design configuration that integrated natural gas reforming with the gasification step directly showed to be the more promising design for the wide range of analyses performed. The Aspen Plus simulation files have been made freely available to the public.

Keywords: Petcoke, Natural gas, Gasification, Fischer-Tropsch, CO₂ capture

1.0 Introduction

1.1 Background

Despite the current trend towards a shift to green and sustainable energy sources with reduced greenhouse gas (GHG) emissions, the use of fossil energy continues to dominate the world's energy mix. According to the 2017 BP statistical review of world energy, a total primary energy of 13.3 billion tonnes of oil equivalent was consumed in 2016 [1] of which fossil energy contributed 86% of the total.

Over 90% of Canada's oil deposit is made up of heavy oil [2] which leaves between 15% to 40% of the oil as residues in the refinery distillation unit [3, 4]. To maximize profit and also meet demands for transportation fuels, refiners further crack these residues in coker units producing unwanted solid carbon material by-product known as petroleum coke (petcoke) [5]. The type of petcoke produced depends on the coker unit used [5]. Fluid and delayed coke are produced in Canada by Syncrude and Suncor respectively [6] with delayed coke getting more industrial attention [7]. Generally, petcoke is classified as either fuel grade or graphite depending on their sulfur content [8] and could be used for wide range of applications such as anode, fuels in kilns, etc. Reports on petcoke availability have ranged between 56 to 150 million tonnes per year (Mt/yr) [4, 8]. Recently, stockpiled petcoke produced in Canada by Syncrude, Suncor, and CNRL near Fort McMurray, Alberta is estimated to be about 100 (Mt/yr) [9] with reasons being due to lack of transportation and carbon sequestration [4]. Such a large amount of solid fuel is sufficient to create dedicated power and chemical production facilities solely running on petcoke.

Therefore, just like coal, petcoke can be used for power generation in supercritical pulverized coal (SCPC) or integrated gasification combined cycle (IGCC) plants since it has a competitive heating value of 34.7 MJ/kg [10] and can be obtained at very low cost since it is a waste product. On the downside, petcoke is a dirty fuel with 5 to 10% higher CO₂ emissions per unit energy produced [4]. Hence, replacing petcoke with coal is obviously not environmentally advisable. However, the conversion of petcoke to make liquid transportation fuels could potentially reduce greenhouse gas emissions by offsetting some petroleum usage. Thus, this study explores petcoke conversion strategies that could be both economically competitive and environmental friendly.

Some studies have examined different commercial plants which use petcoke either alone or in combination with coal for power and chemical productions [11, 12]. However, research on the

techno-economic analysis of petcoke conversion to power, chemicals, and fuels are limited. Orhan et al. [13] carried out a techno-economic analysis of producing power and hydrogen from petcoke. For a petcoke feed rate of 4200 t/day, 437 MW of electricity and 12.87 tonne/hr of hydrogen (also equivalent to 437 MW of energy content) were produced resulting in a thermal efficiency of 25.6% on a lower heating value basis. A preliminary economic analysis was carried out by Jacob Consulting on a 4 Mt/yr petcoke plant that produces either methanol or hydrogen in which the net present value (NPV) was estimated as a function of oil and gas prices [9]. The study showed that there is a business case for using petcoke as a feedstock for fuel production. Similarly, the National Energy Technology Laboratory in the United States Department of Energy (NETL) performed a techno-economic study of converting petcoke to hydrogen, industrial grade steam, fuel gas, power, and liquid fuels [14]. They also concluded that there is a business case for petcoke conversion to fuels under the right market conditions. However, neither study looked at the potential environmental benefits of using waste petcoke as a resource, nor did they examine any potential synergies that could be exploited by combining petcoke with natural gas as feedstock.

Recently, Salkuyeh et al., [15] carried out an optimization study on a petcoke and natural gas polygeneration plant for the production of dimethyl ether (DME), methanol, olefins, and Fischer-Tropsch (FT) liquids. The result of the study showed that market prices strongly determined which of the possible products were the most economically optimal to produce. In addition, it was found that depending on market prices, the economically optimal polygeneration plant used either 20% petcoke (and 80% gas), or no petcoke at all, with the gas-only configuration strongly preferred with the market prices at the time of the study. However, the work only looked at economics and did not consider any potential environmental benefit by using waste petcoke as a resource instead of stockpiling. In addition, the study did not look at petcoke-only designs.

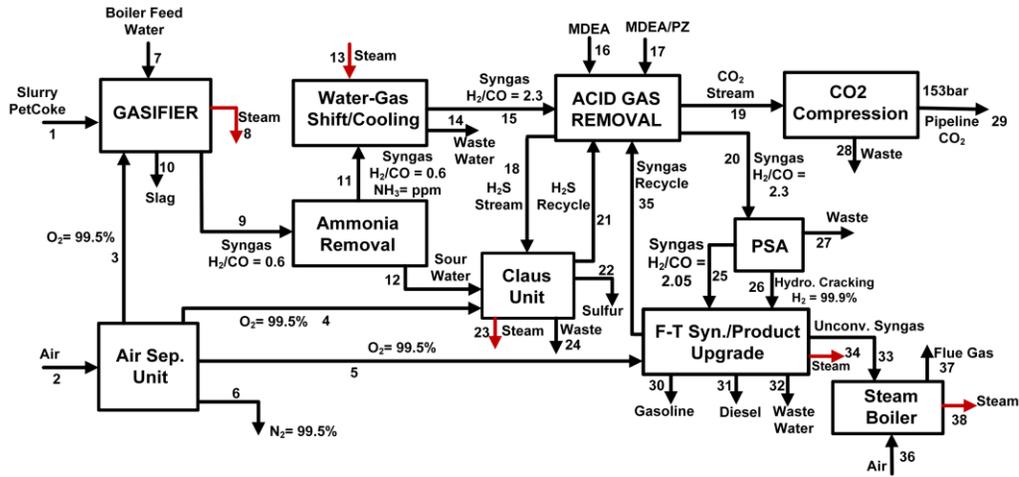
Therefore, this work focuses on the environmental benefits of using waste petcoke for FT liquids production. In this study, different petcoke conversion strategies are proposed as pathways by which petcoke can be converted to FT liquids. The design configurations evaluated are as follows: petcoke standalone gasification (PSG) in which petcoke is the only feedstock; petcoke integrated natural gas reforming (PG-INGR) which integrates petcoke gasification and natural gas reforming in the tubes of the gasifier's radiant syngas cooler; and petcoke external natural gas reforming (PG-

ENGR), which uses petcoke gasification and natural gas reforming as separate units but blends their syngas products together. These designs are adopted from the work of Adams et al. [16]

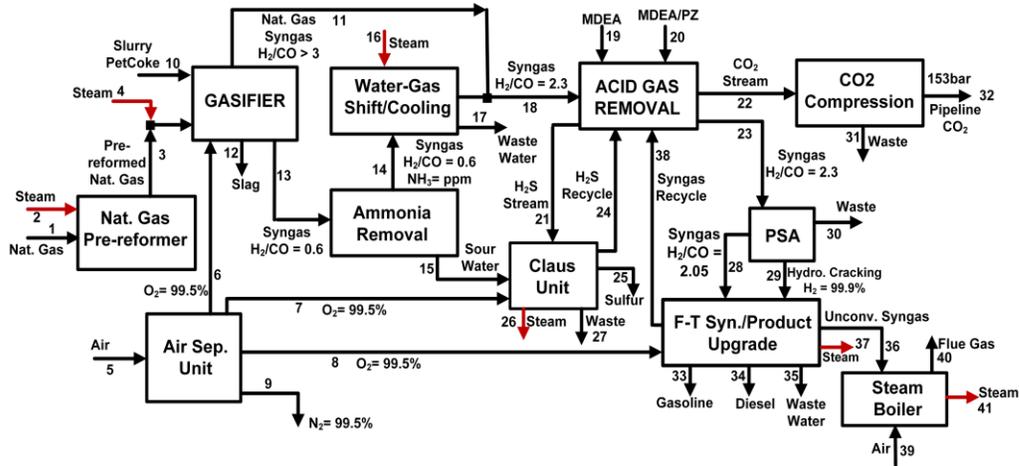
The objective of this paper is to ascertain in detail the economic and environmental performance of the three proposed petcoke conversion strategies. A process flow diagram showing the different conversion strategies is shown in fig 1. A petcoke slurry is gasified in the presence of O_2 (99.5%) to produce syngas with low H_2/CO ratio. Depending on the configuration, either boiler feed water (BFW) or a natural gas/steam mixture is fed through the gasifier's radiant syngas cooler tubes (for natural gas, the tubes are packed with catalyst) providing the cooling duty required to cool the hot gasifier syngas and simultaneously either producing steam or syngas respectively in the process. This distinguishes the PSG and PG-ENGR configurations from the PG-INGR design as the hot gasifier syngas heat is used to drive the endothermic steam natural gas reforming process in PG-INGR instead of making high pressure steam (HPS) in the PSG and PG-ENGR designs.

The gasifier syngas is quenched and flashed to remove entrained impurities and contaminants. Water gas shift and carbonyl sulfide (COS) hydrolysis are employed to raise the H_2/CO ratio and convert COS to H_2S respectively. Natural gas derived syngas from the PG-INGR or PG-ENGR design is mixed with the shifted gasifier syngas and sent to the methyl di-ethanolamine (MDEA) based acid gas removal unit for H_2S and CO_2 removal. The absorbed H_2S is sent to the Claus unit for sulfur production while aqueous MDEA enriched with piperazine is used to capture CO_2 which is sent to the CO_2 compression unit for sequestration. A small amount of H_2 is extracted from the syngas via a pressure swing adsorber (PSA) unit for use in a downstream hydrocracker. The syngas is then sent to the FT reactor where it is converted to FT syncrude. The syncrude is distilled and hydrocracked to produce gasoline and diesel fractions. To promote the formation of liquids, 90% of the unconverted hydrocarbons are recycled back to the FT reactor while the remaining is combusted for HPS generation. For comparison, variants of each of these three designs were considered with no CO_2 capture and sequestration (CCS), resulting to a total of six designs considered in this analysis.

PSG



PG-INGR



PG-ENGR

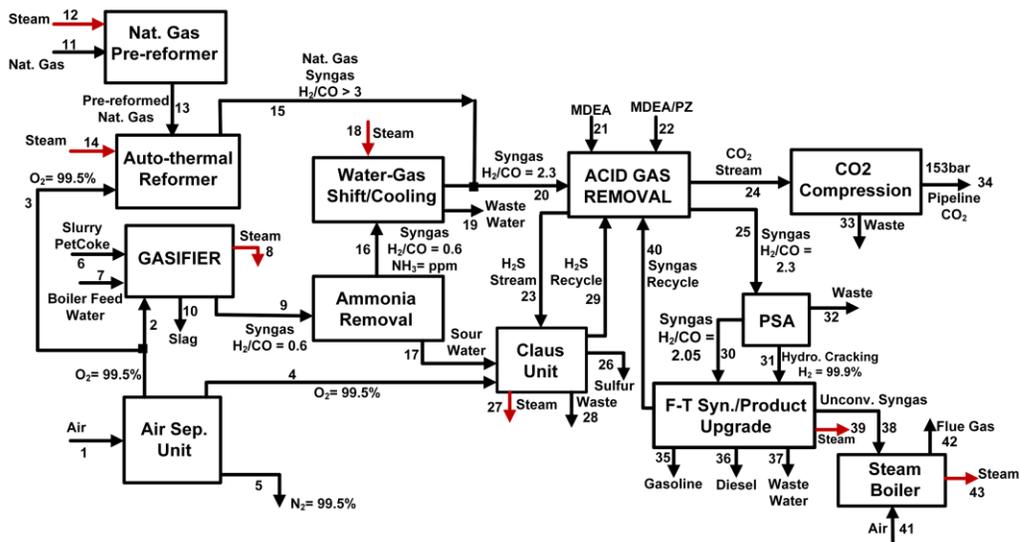


Figure 1: Process flow diagrams for the three petcoke conversion to liquid fuels strategies.

2.0 Methodology

2.1 Process simulation/assumptions

This paper considers the use of delayed coke produced in Alberta, Canada and conventional pipeline natural gas as the feedstocks that is to be converted to liquid fuels. Based on the NETL petcoke study [14], the petcoke feed rate is 219 t/hr (dry basis) with the natural gas feed rate sized according to the amount of radiant heat recovered in the gasifier that is available to drive the endothermic natural gas reforming reaction. The properties of the feedstock are shown in table 1.

Table 1: Delayed coke analysis [10] and Natural gas composition [17]

Delayed coke			
HHV (MJ/kg)	34.7		
Ultimate analysis (wt. % dry)			
C	84.9	Cl	0
H	3.9	Ash	3.1
N	1.3	O (diff)	0.8
S	6		
Proximate analysis (wt. %)			
Moisture	1.8	Fixed carbon	83.3
Volatile matter	11.9	Ash	3
Natural gas			
HHV (MJ/kg)	52.97		
Components (%mole)			
CH ₄	93.9	CO ₂	1.0
C ₂ H ₆	3.2	C ₄ H ₁₀	0.4
N ₂	0.8	C ₃ H ₆	0.7

The simulation of the 3 petcoke conversion strategies was carried out in Aspen Plus v10 except for the MDEA based H₂S and CO₂ removal sections which were modeled in ProMax. The Peng-Robinson with Boston-Mathias (PR-BM) equation of state was used (which is consistent with our previous work [16]) with a few exceptions. The Amine package (in ProMax) was used for the ProMax MDEA model while the CO₂ compression unit in Aspen Plus used the Predictive Redlich-Soave-Kwong (PRSK) model which was shown in prior work to be superior at high pressures [18]. For the ammonia-water system, the PR-BM, PSRK, and the Electrolyte Non-random Two Liquid (ElectNRTL) model were evaluated and compared against the experimental work of Guillevic et

al. [19] to determine the best candidate model for the $\text{NH}_3\text{-H}_2\text{O}$ vapor-liquid equilibrium system as shown in figure 2. Both PSRK and PR-BM are about equally good; hence PR-BM was chosen to avoid model consistency issues with the rest of the flowsheet.

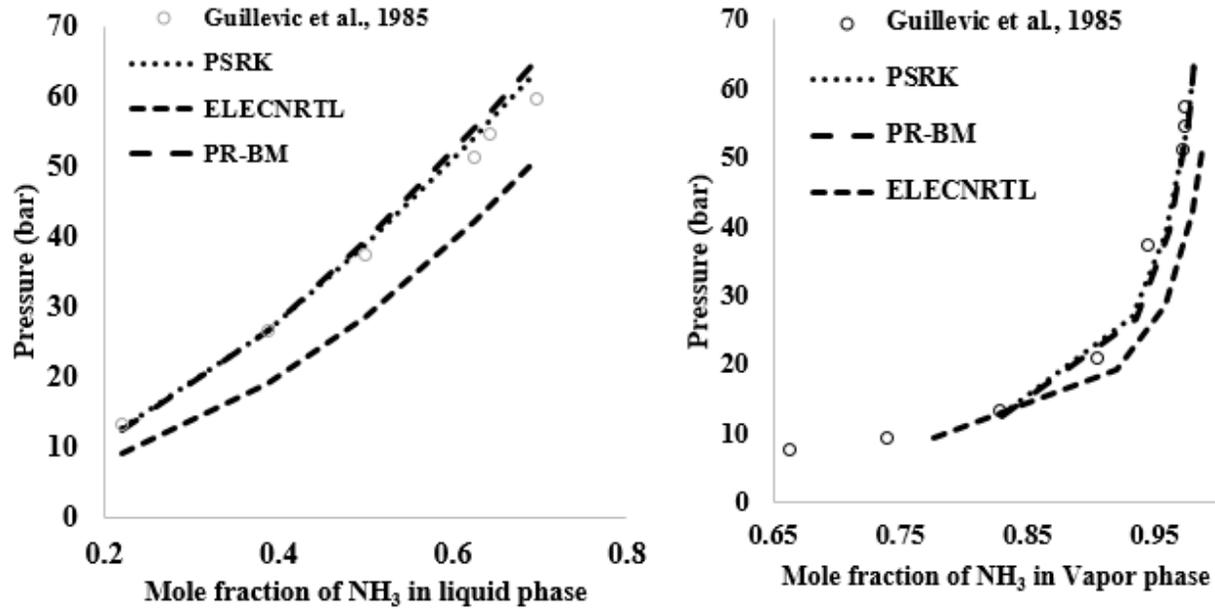


Figure 2: Validation of vapor-liquid equilibrium mixtures of $\text{NH}_3\text{-H}_2\text{O}$ system with three different models.

The Aspen Plus APV100 Pure 36 and Solids databases were employed for specifying the components: Conventional (CO , CO_2 , H_2 , O_2 , H_2O , N_2 , Ar , NH_3 , H_2S , NO , NO_2 , SO_2 , SO_3 , S_2 , S_3 , S_4 , S_5 , S_6 , S_7 , S_8 , $\text{C}_1\text{-C}_{30}$), Solids (C , S), and non-conventionals (petcoke, slag, ash, char). Similar to Adams et al. [16], all C_{30+} hydrocarbons were lumped as follows: C_{32} represents $\text{C}_{31}\text{-C}_{33}$, C_{36} represents $\text{C}_{34}\text{-C}_{39}$ while $\text{C}_{40}\text{-C}_{64}$ are pseudo-components specified to accurately represent the FT products using the normal boiling point, density, and molecular weights based on API gravity. Details of the models operating parameters and assumptions are shown in table 2.

Table 2: Model operating parameters and assumptions

Main design parameters	
Unit	Parameters
ASU	Oxygen purity (99.5%) @ 32 °C, P = 13bar Slurry water/ petcoke (44w%/56w%)
Gasifier	Two train E-Gas Gasifier Exit conditions: T = 1426 °C, P = 55 bar
Water Gas Shift	Low Temp adiabatic reactor, T: 207 °C High Temp adiabatic reactor, T: 425 °C
Acid Gas Removal	COS hydrolysis adiabatic reactor T:177 °C Conversion >> 99% MDEA H ₂ S removal: T = 40 °C, P = 5.5 bar MDEA/piperazine CO ₂ removal: T = 40 °C, P = 30 bar
CO ₂ Compression	Multistage compressor with intercoolers CO ₂ Purity (99.5%) T = 26 °C, P = 153 bar
Sulfur Recovery (Claus)	Split flow [20] (H ₂ S > 15%), Furnace (T:950 °C)
PSA	Hydrogen (99.9%)
F-T/Product Upgrade	F-T Slurry reactor: T = 220 °C, P = 30 bar CO conversion: 80%
Cooling Tower	Product ASTM spec (95% vol): gasoline = 170 °C, diesel = 340 °C Wet bulb temp: 11 °C, Approach temp: 5 °C, cooling water range 11 °C Cooling water inlet: 16 °C
Assumptions	
Minimum temperature approach in heat exchanger	5 °C
Low pressure steam	4 bar, 204 °C
Medium pressure steam	12 bar, 300 °C
High pressure steam	50 bar, 480 °C
Fired heat	1000 °C
Chilled water	4 °C
Isentropic efficiency in compressors	80%
Mechanical efficiency in compressors	100%
Maximum permitted pressure ratio in compressors	5
Pump efficiency	80%

2.2 Air Separation Unit

Oxygen needed for the process is produced by compression, cooling, liquefaction and distillation of air in the overall cryogenic separation unit. This separation is enhanced by the boiling points

difference which exists among air constituents (nitrogen, oxygen, carbon dioxide, argon, helium, neon, krypton and xenon). Atmospheric air is trapped and compressed to a discharge pressure of 1.3 MPa in a multi-stage with intercooler (at 31 °C) compressor allowing for removal of condensed vapor. In this paper, ASU separation coefficients were adopted from the work of [17] which was modeled in Aspen Plus using SEP and calculator blocks to compute and implement the mass balances that result in the production of oxygen at 99.5% purity. In this work, the ASU parasitic load which accounts for the sum total of the cryogenic section parasitic load and the boost compression of portions of the produced O₂ to the different pressure levels needed in the plant was estimated to be 0.41MW/t/hr of O₂.

2.3 Syngas Production

2.3.1 PSG

Delayed petcoke delivered at the plant gate is ground and mixed with water to form slurry (H₂O: petcoke, 44wt%/56wt%) prior to being fed to the petcoke gasifier similar to the Wabash E-Gas gasifier [21] that processes petcoke. Gasification reaction comprises of pyrolysis, volatile combustion, char gasification, and sulfur reaction of which the product depends on the particular fuel characteristic. The slurry feed is gasified with oxygen (99.5% purity) at 1426 °C and 5.6 MPa to produce syngas consisting primarily of H₂, CO, CO₂, and other impurities [17, 22]. To accurately represent the overall gasification process, the pyrolysis (breakdown) of the solid fuel to elemental species is first modeled as petcoke decomposition occurring at 550 °C [23] in an RYield reactor using calculator block to estimate the components yields which is based on fuel composition. Then followed by the actual gasification reactions such as volatile combustion, char gasification, and sulfur reactions in the petcoke gasifier modeled in Aspen Plus using RGibbs reactor which follows a restricted chemical equilibrium approach to produce syngas.

Oxygen is fed to the reactor in such a way that the desired reactor temperature is maintained during the gasification process. The heat of fusion of ash (230 kJ/kg) [24] and heat loss to the environment (assumed to be 1% of HHV_{petcoke}) during gasification were considered for the energy balance of the gasifier. Boiler feed water (BFW) is used to provide the cooling duty required by the hot gasifier syngas cooling it to 760 °C in the radiant syngas cooler (RSC) producing HPS [21, 25]. Conversion of carbon in petcoke was assumed to be 99% similar to the petcoke gasification test

of Wabash River [21]. The unconverted carbon in the feed was considered to be ash in addition to trace metals such as vanadium and nickel which exists the gasifier as slag [23]. To remove the slag entrained in the syngas, the gas is passed through a water-quench pool at an adiabatic saturation temperature of about 200 °C. Ammonia removal from syngas which deactivates the FT catalyst [26] was carried out based its high solubility in the NH₃-H₂O system reducing it to 10 ppm limit [27]. The NH₃ rich water termed “sour water” is sent to the Claus unit for NH₃ destruction [28].

2.3.2 Natural gas reforming

Pipeline natural gas is delivered to the plant gate at 30 °C and 30 bar with the composition as shown in table 1. Due to the presence of higher hydrocarbons, the gas is adiabatically pre-reformed at 450 °C to achieve up to 99% of all >CH₄ hydrocarbons. This design applies to both the PG-INGR and PG-ENGR configurations.

2.3.2.1 PG-INGR configuration

Steam methane reforming is used to provide the cooling duty required by the hot gasifier syngas. This is achieved by sending the pre-reformed natural gas and steam through the RSC tubes packed with alumina catalyst thereby reforming the natural gas for additional syngas production. Gasifier syngas leaves at 760 °C which is equivalent to 216 MW cooling duty. To determine the natural gas and steam feed rate (for at least 80% methane conversion) that will provide the required cooling duty, a first principles model of an integrated petcoke gasification and steam methane reformer based on the work of Ghouse et al. [29] was used in gProms. The model is multi-scale and considers spatial gradients temperature, concentration, and pressure of the gases in both sides of the tubes. It also models the effects diffusion within the catalyst particles themselves to the millimeter scale, and is approximately 100,000 equations in size (see [29] for details). In addition to methane conversion, the tube exit temperature, pressure drop, and steam conversion were also determined with this model. The tube syngas has a H₂/CO ratio > 3 which is mixed with the gasifier syngas for downstream conversion.

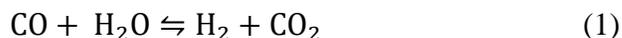
2.3.2.2 PG-ENGR configuration

Similar to the work of Salkuyeh et al .[15], this design explores the performance of combining petcoke and natural gas as feedstock in the conversion strategies by reforming natural gas in an auto-thermal reformer. For comparison, the same amount of pre-reformed natural gas is fed to an

auto-thermal reformer operating at 950 °C and 30 bar. Oxygen is used for in-situ oxidation of the methane thereby providing the heat requirement of the process while the steam to carbon ratio was varied to obtain the desired H₂/CO ratio > 3. The syngas generated in this process is mixed with the gasifier syngas for subsequent downstream conversion to FT liquids.

2.4 Syngas Shifting

Water gas shift (WGS) is employed to convert the excess CO in the petcoke derived syngas to achieve the desired H₂/CO ratio. Typical of industrial processes, both the high temperature water gas shift (HTWGS) and low temperature water gas shift (LTWGS) reactors operating adiabatically were used in series due to equilibrium limitations of the HTWGS [30]. The HTWGS operates at about 425°C in the presence of chromium or copper promoted iron-based catalysts followed by the LTWGS reactor operating at 260°C in the presence of copper-zinc-aluminum completing the shift process [31] to the desired H₂/CO ratio of 2.3. The excess H₂ is used in the hydrocracking unit. In addition to the CO conversion in the WGS reactors, COS conversion to H₂S also takes place simultaneously. Both reactors were modeled in Aspen Plus using an equilibrium model (REquil) with these reactions:



To achieve up to 99% of COS conversion, equilibrium catalytic hydrolysis of COS in the presence of activated alumina catalyst was employed [32]. Finally, the syngas is cooled to 40°C and flashed to remove waste water while the syngas is sent to the acid gas removal unit.

2.5 Acid Gas Removal

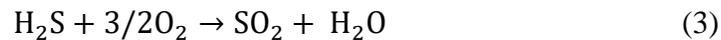
Acid gas removal was simulated in ProMax using MDEA to remove H₂S and CO₂ from the syngas. Syngas is fed through the bottom of the H₂S absorber operating at 40 °C in a counter-current fashion with the MDEA/H₂O (50%:50%) solvent [33, 34]. Although H₂S and CO₂ are highly soluble in MDEA, the solubility of H₂S proceeds at a very fast rate compared to CO₂ [35] which ensures minimal pickup of CO₂ in the H₂S absorber. The H₂S absorber was designed to achieve 98% H₂S removal efficiency with a solvent to feed ratio of 1.85. Syngas exiting the top of the absorber is cooled, flashed to remove some of the entrained water, and sent to the CO₂ absorber unit while the bottoms product (rich MDEA solution) exiting the bottom of the absorber is regenerated in the H₂S stripping column operating at 2 bar. Exiting the top of the H₂S stripper is a

stream containing 15% H₂S which is sent to the Claus unit for split flow sulfur recovery process [28] while the bottoms stream made up of the regenerated solvent is pumped back to the top of the H₂S absorber.

In the CO₂ absorber, the capture of CO₂ from the syngas is promoted by the aid of piperazine [20, 36] which enhances the overall absorption of CO₂ given its slow reactivity in MDEA [34]. A solvent mixture of (50% wt:45% wt:5% wt) H₂O/MDEA/piperazine was employed [20]. Apart from the use of piperazine, the process is similar to the H₂S absorption process. The absorber was designed to capture 90% CO₂ which is typical for solvent based carbon capture [37, 38] with a solvent to feed ratio of 2.98. The syngas exiting the CO₂ absorber is sent through the PSA to the FT unit while the CO₂ stream is sent to the CO₂ compression unit.

2.6 Claus Process

Hydrogen sulfide from the AGU is catalytically converted to elemental sulfur in the Claus process. The basic reactions comprise the partial oxidation of H₂S to produce SO₂ followed by the reaction of the unconverted H₂S with SO₂ as shown in the reactions:



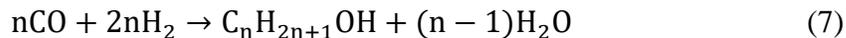
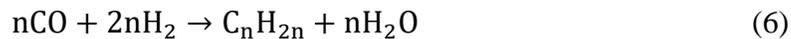
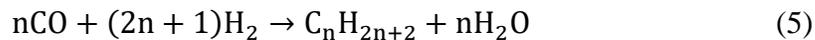
Combustion of acid gas and sour water in the presence of limited oxygen in a Claus furnace takes place at 950 °C [28] to generate gas mixture with the desired stoichiometric coefficient of 2:1 for H₂S and SO₂ respectively for subsequent conversion to sulfur and water [39, 40]. Some elemental sulfur is produced at the furnace with the sulfur reactions modeled as an equilibrium reaction with temperature approach. Exiting the furnace is a hot stream containing predominantly elemental sulfur that is cooled in the waste heat boiler (WHB) recovering heat that is used for HPS generation [39]. The stream leaving the WHB is condensed and reheated to 210 °C upstream the catalytic reactors [28]. Two stage catalytic reactors with intermediate condensers and heaters were used [28, 39] for this process achieving a sulfur recovery of 96% [41]. The recovered sulfur is cooled and stored in sulfur pit for subsequent sale while the unconverted H₂S is recycled back to the MDEA unit.

2.7 Pressure Swing Adsorption

Prior to the FT reactor, PSA is used to recover 99.99% pure hydrogen from the syngas stream. Since hydrogen is the desired component, adsorbent with low binding force with hydrogen due to its low polarity and very high volatile is used. Detailed modeling of the PSA is not within the scope of this work and was represented using a SEP block in Aspen Plus by setting the hydrogen recovery to 99.99%.

2.8 Fischer-Tropsch Synthesis/Product Upgrade

Liquid fuels production takes place in the low temperature FT slurry reactor in the presence of cobalt catalyst. The choice of reactor, temperature and catalyst is to promote the formation of diesel fractions of the fuel. Syngas entering the FT slurry reactor with the desired H₂ to CO ratio of 2.05 is raised to 240 °C and 30 bar with the reactions proceeding as:



A single pass CO conversion of 80% was assumed which is typical of the slurry phase reactors [42]. Theoretically, the production of diesel fraction of liquid fuels is promoted by higher α value. Since values for industrial FT reactors are characterized between 0.65 and 0.95 [43], a high value (0.92) was chosen. The product distribution is based on the work of Adams et al. [16]. The syncrude produced in the FT reactor is cooled, decanted to remove water, and sent to the product upgrading unit. For brevity, the detailed modeling of the hydrocracking of heavy hydrocarbons, product upgrade, and product distribution to produce gasoline and diesel can be found in Adams et al. [16]. In order to maximize the production of liquid fuels, 90% of the unconverted hydrocarbons are recycled to the FT reactor via an auto-thermal reactor which reforms the unconverted hydrocarbons to H₂ and CO while the remaining 10% was used for HPS generation.

2.9 Heat Integration (Utilities and cooling tower system)

Plant wide utility management was designed and optimized using Aspen Energy Analyzer to maximize heat recovery; thus, minimizing energy requirement (MER). The heat exchanger network that meets the MER was designed using pinch analysis. All process streams with their

process conditions were exported from Aspen Plus to Aspen Energy Analyzer (AEA). Assuming a minimum approach temperature (ΔT_{\min}) of 5 °C, the composite curves (CC) and grand composite curves (GCC) were constructed as depicted in figure 3 showing the pinch temperatures and maximum possible heat that can be recovered by process to process heat exchange.

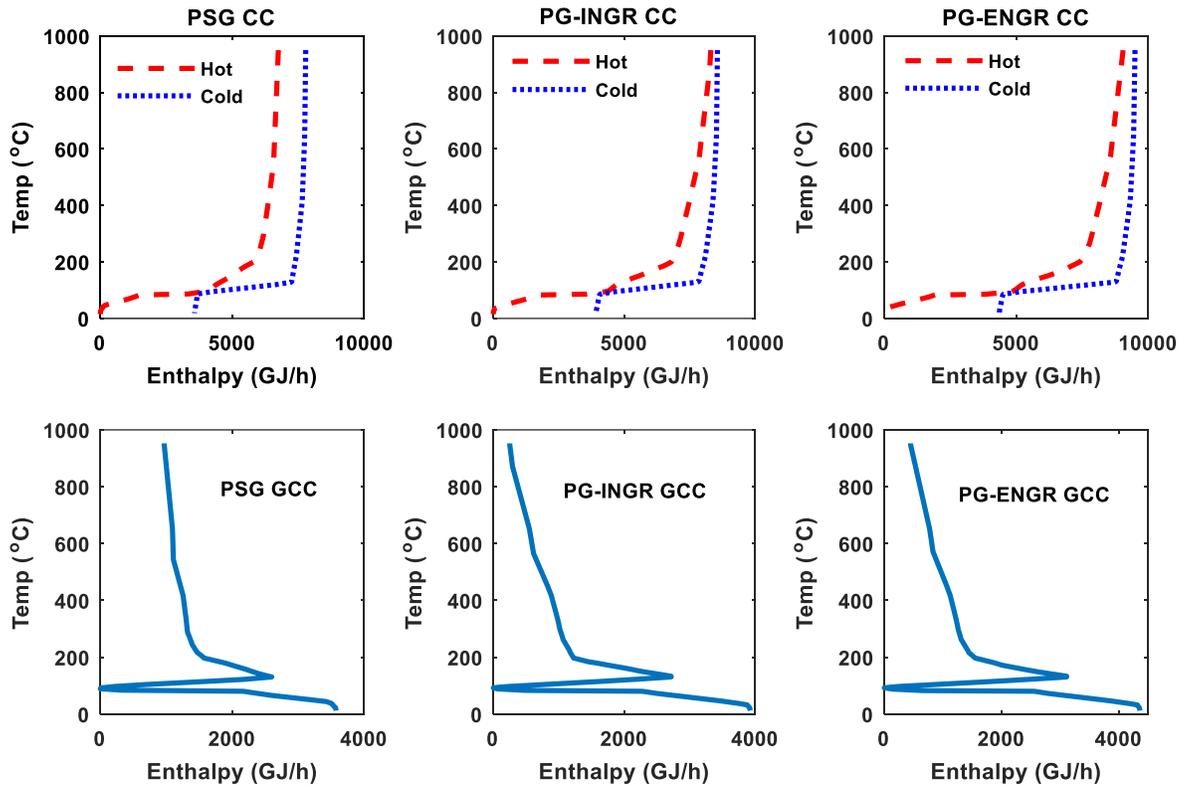


Figure 3: Composite and Grand composite curves for the three petcoke conversion strategies at $\Delta T_{\min} = 5 \text{ }^{\circ}\text{C}$

The conditions of the utility streams used for the design are shown in table 2. Utility allocation was based on the grand composite curve (GCC) utility allocation method which employs a heuristic that maximizes the use of the cheapest utility [44]. AEA proposes multiple near-optimal designs of the HEN by solving the MILP minimizing the objective function; total annualized cost (TAC). The design with the smallest TAC was chosen as the best candidate design for each of the configuration strategies.

The cooling water requirement of the process was designed using a mechanical draft evaporative cooling tower system with an approach temperature of 5 °C and cooling range of 11 °C [17]. The estimation of the amount of cooling tower makeup followed a correlation in [45] with cycles of

concentration, and evaporative and drift losses of 5, 0.8%, and 0.001% respectively. The cooling tower pump and the fan together accounts for the tower electrical power consumption, which was calculated using correlations from Turton et al., [45] using a pump efficiency of 80% and pressure drop of 2.6 bar.

2.10 Techno-economic Analysis

A techno-economic analysis (TEA) of the 3 petcoke conversion strategies to liquid fuels was conducted to determine the most profitable design. Detailed economic assumptions are shown in table 4 which was made to be consistent with the NETL petcoke gasification study [14]. The discounted cash flow rate of return approach was used to estimate the net present value (NPV). Since diesel is the main product of the process, the minimum diesel selling price (MDSP) was also calculated as the selling price which results in a NPV of zero.

Table 4: Economic assumptions

Parameter	Value	Ref
Plant life (yrs)	30	[16]
Construction period (yrs)	2.5	
Plant loan (yrs)	30	
Plant loan interests	9.50%	[46]
Debit/Equity (%)	80/20	[14]
Tax Rate	40	[46]
Rate of Return	12%	[14]
Depreciation Method	MACRS	
Working capital	5% TPC	[47]
Length of start-up	20	
Operating Hours	8000	

With the aid of the mass and energy balance, the equipment costs for the three conversion strategies were estimated using a combination of literature and Aspen Process Economic Analyzer (APEA v10) except the gasifier of the PG-INGR configuration. Because no economic data exist for the integrated gasifier (since it has not been commercialized), it was assumed that the integrated gasifier costs 50% more than a gasifier with a typical radiant syngas cooler of the same capacity as reported by the NETL [17]. This parameter was subjected to a sensitivity analysis to ascertain its effect on the NPV. Plant wide heat exchanger costs were obtained from the AEA results. All estimated equipment costs were scaled up to US\$2017 using the chemical engineering plant cost

indices [48]. Details of the capital cost estimation can be found in the attached supplementary information. Variable operating costs (feedstock, catalysts, utility) and product prices were obtained from literature reports and market prices respectively which were scaled to \$2017 while the fixed operating costs (labor, maintenance, and overhead) were calculated using the method given by Seider et al. [49]. The variable and fixed operating costs are detailed in table 5.

Table 5: Fixed and Variable operating costs based on market and literature data.

Fixed costs (Labor, Maintenance, and Overheads)		Ref
Direct wages and benefits (DW&B)	32 operators/shift	[49]
Direct salaries and benefits	15% of DW&B	[49]
Operating supplies and services	6% of DW&B	[49]
Tech. assistance to manufacturing	\$60,000 base for 5 shifts	[49]
Control laboratory	\$65,000 base for 5 shifts	[49]
Wages and benefits (MW&B)	4.5% of TDEC	[49]
Salaries and benefits	25% of MW&B	[49]
Materials and services	100% of MW&B	[49]
Maintenance overhead	25% of MW&B	[49]
Operating Overhead	22.8% of M&O-SW&B	[49]
Property Insur. & Tax	2% of TDEC	[49]
Feedstock, product, and byproducts prices		
Petcoke (Feedcost)	0.000 \$/tonne	[14]
Natural gas	\$1.4/MMBtu	
Sulfur price	\$70/ton	[50]
Gasoline	\$1.826/gal	[51]
Diesel	\$1.852/gal	[52]
Utility		
Cooling tower Water	\$0.0148/tonne	[45]
Chilling Water	\$4.00/GJ	[49]
Boiler Feed Water	\$0.5/tonne	[49]
Electricity	\$38/MWh	
LP Steam	\$7.78/GJ	[45]
MP Steam	\$8.22/GJ	[45]
HP Steam	\$9.83/GJ	[45]
Fired heat	\$7.5/GJ	[45]
Solvents, Catalysts & Wastes		
Waste Water Treatment	\$0.528/tonne	[47]
MDEA Price	\$244/tonne	[53]
Piperazine	\$244/tonne	Assumed
Ash	\$15.45/ton	[17]
WGS Catalyst	\$63.889/kg	[17]
Claus Catalyst	\$125/ft ³	[17]

COS Catalyst	\$2308.4/m ³	[17]
FT Catalyst	\$35/kg	[54]
Product upgrade Catalyst	\$56.36/kg	[55]
CO ₂ Emission	\$50/tonne	[16]

3.0 Results and discussion

3.1 Process simulation

The converged Aspen Plus simulation files for all six cases are available for download on the digital archive at PSEcommunity.org¹. The results of the six petcoke conversion strategies (with CCS and w/o CCS) are briefly summarized in table 6 detailing the feed rates, total electricity consumption, fuels production rates, by-product rate, and cradle to plant exit life cycle GHG emissions. Also, feed carbon, fuel, and energy efficiencies were computed. It is noteworthy to observe the amount of natural gas feed to the PG-INGR and PG-ENGR designs. This is based on the 216 MW of heat recovered in the gasifier radiant cooler which was used to drive the natural gas to 80% conversion.

Table 6: Summary of the different design performance

	PSG	PSG	PG-INGR	PG-INGR	PG-ENGR	PG-ENGR
	Yes	No	Yes	No	Yes	No
Petcoke Feed rate (tonnes/h)	218.7	218.7	218.7	218.7	218.7	218.7
Gasifier Radiant Heat Recovered (MW)	216	216	216	216	216	216
Natural Gas (tonnes/hr)	-	-	52.3	52.3	52.3	52.3
Total Electricity consumed (MW)	232.2	189.4	272.7	239.2	315.0	270.5
Fuel Efficiency (HHV%)	43.4	43.4	51.9	51.9	46.2	46.2
Energy Efficiency (HHV%)	33.4	36.4	42.6	44.6	36.6	37.9
Carbon Efficiency (%)	32.2	32.2	43.7	43.7	38.9	38.9
Gasoline produced (ML/yr)	232.2	232.2	386.8	386.8	344.1	344.1
Distillate produced (ML/yr)	627.3	627.3	1025.9	1025.9	914.4	914.4
Sulfur produced (ktonnes/yr)	99.8	99.8	99.6	99.6	99.1	99.1
CO ₂ sequestered (Mtonnes/yr)	3.5	-	3.4	-	3.7	-
Direct GHG emitted (MtonnesCO ₂ eq/yr)	0.1	3.6	0.2	3.6	0.2	3.9
Indirect GHG emitted (MtonnesCO ₂ eq/yr)	0.8	0.4	0.9	0.7	1.1	0.9
Direct GHG emitted (kgCO ₂ eq/GJ)	2.6	67.8	2.5	41.7	2.4	50.7
Indirect GHG emitted (kgCO ₂ eq/GJ)	15.1	8.4	10.7	7.9	14.3	12.2
Total GHG Emission (kgCO ₂ eq/GJ)	17.7	76.2	13.2	49.3	16.6	62.9

¹ The permanent link to the files is: <http://psecommunity.org/simfiles/okekeadams2018.zip>

Comparing the three designs with CCS, the PG-ENGR design consumed the highest amount of electricity, 36% more than PGS and 16% more than PG-INGR. This high amount of power consumption in the PG-ENGR design is because of the high parasitic load of the ASU in providing the oxygen needed to drive the auto-thermal reformer. Without CCS, there is an 18%, 12%, and 14% reduction in electricity demand for the PGS, PG-INGR, and PG-ENGR designs respectively which when compared to the CCS plant. Liquid fuels production for the PG-INGR and PG-ENGR conversion strategies that combined petcoke and natural gas are 65% and 46% respectively higher than the PGS which converts only petcoke, due in large part to the much larger amount of total feedstock used. However, PG-INGR produces 12% more liquid fuels than PG-ENGR even though they both use the same amount of feedstock, signifying that the PG-INGR design has much improved conversion capability.

3.2 Process Emissions

3.2.1 CO₂ capture and emissions

The direct and indirect CO₂ emissions of the configuration for the CCS and non-CCS enabled scenarios are shown in figure 4. The direct emissions consist of all the process GHG emissions from the plant entry to the plant exit while the indirect emissions accounts for all cradle to plant entry GHG emissions. The electricity emission used in this study is the average Ontario electricity mix emission of 52.76 gCO₂eq/kWh [56]. GHG emissions for natural gas extraction and transportation, and utility emissions were obtained from NETL [57] and EPA [58] respectively. In this study, the indirect emissions of petcoke production was taken to be zero which is reasonable as it is an undesired waste product of refinery operation (one does not refine oil to get the petcoke); thus, all petroleum extraction and refining emissions are attributed to the useful refinery products instead.

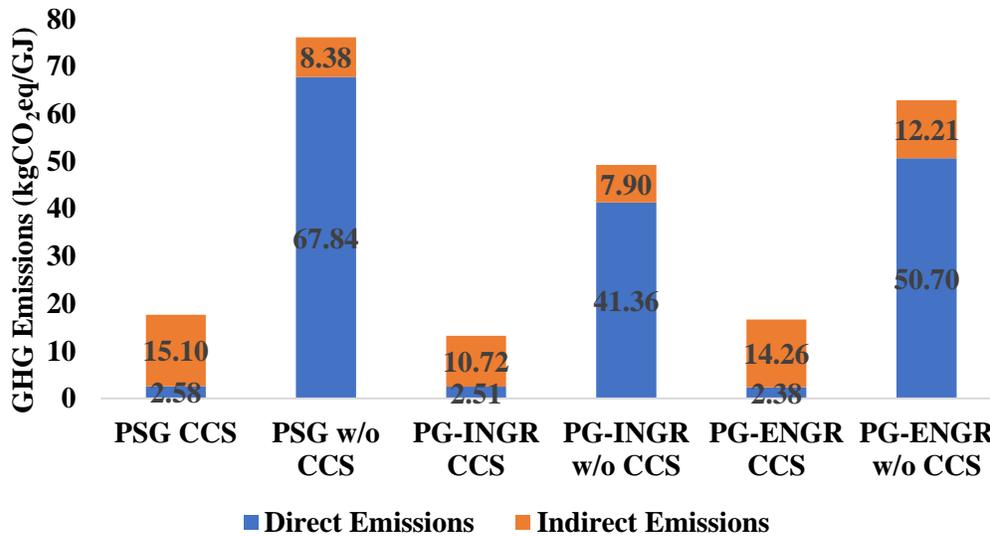


Figure 4: Cradle-To-Product GHG emissions for the different designs

Fig. 4 shows a higher indirect emission of the CCS plants compared to their non-CCS counterpart due to the parasitic CCS technology. On an absolute basis, the PG-INGR design has 59% and 19% more direct emissions than the PSG and PG-ENGR designs (see table 6). However, when expressed per GJ of liquids produced, the CCS plants have almost the same amount of direct emission whereas the PG-INGR has approximately 25-29% lower indirect emissions compared to the PSG and PG-ENGR designs. Similarly, total cradle to plant exit gate GHG emissions for PG-INGR are 20-25% lower than the PSG and PG-ENGR designs. Without CCS, although there is a significant drop in indirect emissions across the designs due to less parasitic load, the direct emissions of the PSG, PG-INGR, and PG-ENGR designs are 16-26 times higher than their CCS-enabled counterparts. Overall, the PG-INGR design emits the least total life cycle CO₂ even when operated without CCS.

3.2.3 Cost of CO₂ Avoided

An important metric for comparing different designs and processes for the purpose of capturing or reducing CO₂ emissions compared to a reference plant (typically a plant that represents the status quo without carbon capture technology) is the cost of CO₂ avoided (CCA) [38]. For this study, a conventional crude oil refinery is used as the reference plant as it produces the same product. Therefore, the CCA is defined as:

$$CCA = \frac{(TPC_{CCS_plant} - TPC_{Refinery})}{(GHG_{Refinery} - GHG_{CCS_plant})}$$

where TPC_{CCS_plant} and GHG_{CCS_plant} are total product cost (TPC in \$/GJ) and total cradle to plant exit gate emissions (tonneCO_{2e}/GJ) of a liquid fuels plant with CCS respectively while $TPC_{Refinery}$ and $GHG_{Refinery}$ are total product cost (TPC in \$/GJ) and total cradle to plant gate exit emissions (tonneCO_{2e}/GJ) of a refinery without CCS respectively.

The refinery cradle to plant exit gate GHG emissions used in this work is 31.81 kgCO_{2eq}/GJ which is consistent with that from GREET model [59] and the NETL [60]. This included the total direct and indirect emissions of a conventional crude oil extraction, transportation to refinery, and emissions for production of 1 MJ of diesel and gasoline respectively. The GHG emissions computed followed the International Panel on Climate Change (IPCC) 100-year metric. Considering only diesel and gasoline refinery emissions helps to ensure product emission consistency. To calculate the TPC, the capital investment (M\$) was annualized using the Smith et al. [61] annualization factor (AF):

$$AF = \frac{i(1+i)^n}{(1+i)^n - 1}$$

where i is the rate of return (%) and n is the plant life (y).

The annualized capital investment (M\$/yr) was added to the plants' annual operating cost (M\$/yr), divided by the annual production capacity (in GJ/yr) to obtain the TPC of the process (in \$/GJ). Total product cost of the refinery was estimated using the reported wholesale prices of diesel [52] and gasoline [51] in the US. Diesel and gasoline were assumed to be the only products of the refinery accounting for 62% and 38% respectively which is similar to the fuel fractions obtained in this work. Since the reported refiner's plant gate prices for the products usually includes refinery margins, which have been reported to be up to \$5.5/bbl based on the current crude oil price [62], the margin was factored into the refiner's wholesale price to obtain a refinery total product cost of \$14.72/GJ which was used as the TPC of the refinery.

Table 7: Cost of CO₂ Avoided Calculation for the three configurations with CCS enabled

	PSG	PG-INGR	PG-ENGR
CCS-Enabled	Yes	Yes	Yes
Total capital Cost (M\$)	1116	1382	1370
Annualized capital Cost (M\$/yr)	294	365	361
Operating Cost (M\$/yr)	235	345	315
Total Product (MGJ/yr)	26.4	43.3	38.5
Total Product cost (\$/GJ)	20.1	16.4	17.6
GHG (kgCO ₂ eq/GJ)	17.7	13.2	16.6
CCA (\$/tonneCO ₂ eq)	379	90.1	189

Table 7 shows the calculated CCA in \$/tonneCO₂eq for the different configurations. Considering the high cost (\$/GJ) and emissions of the PGS design, it clearly is not a good choice for environmental purposes when compared to the petcoke and natural gas designs as its CCA is approximately 2 to 4 times that of the PG-ENGR and PG-INGR designs, respectively. Also, the CCA of the PG-ENGR design is 2.1 times that of the PG-INGR design. Therefore, the integrated gas reforming strategy is clearly the best option in terms of environmental emissions.

3.3 Process Efficiencies

3.3.1 Carbon efficiency

To further study the performance of the each of the design configurations, the carbon efficiency, which is the percentage of carbon in feedstock which ends as useful product, was evaluated. The carbon efficiency (η_{carbon}) is defined as:

$$\eta_{carbon} = \frac{Diesel_{carbon} + Gasoline_{carbon}}{Fuel_{carbon}}$$

where $Diesel_{carbon}$, $Gasoline_{carbon}$, and $Fuel_{carbon}$ are the mass of carbon atoms in diesel product, gasoline product, and fuels (petcoke only or petcoke and natural gas) depending on the design employed. Fig. 5 shows the percentages of carbon in product, carbon sequestered, and carbon emitted. The PG-INGR configuration (with or without CCS) has the highest carbon efficiency of 43.7% which is 11.5 and 4.80 percentage-points larger compared to the PSG and PG-ENGR designs respectively.

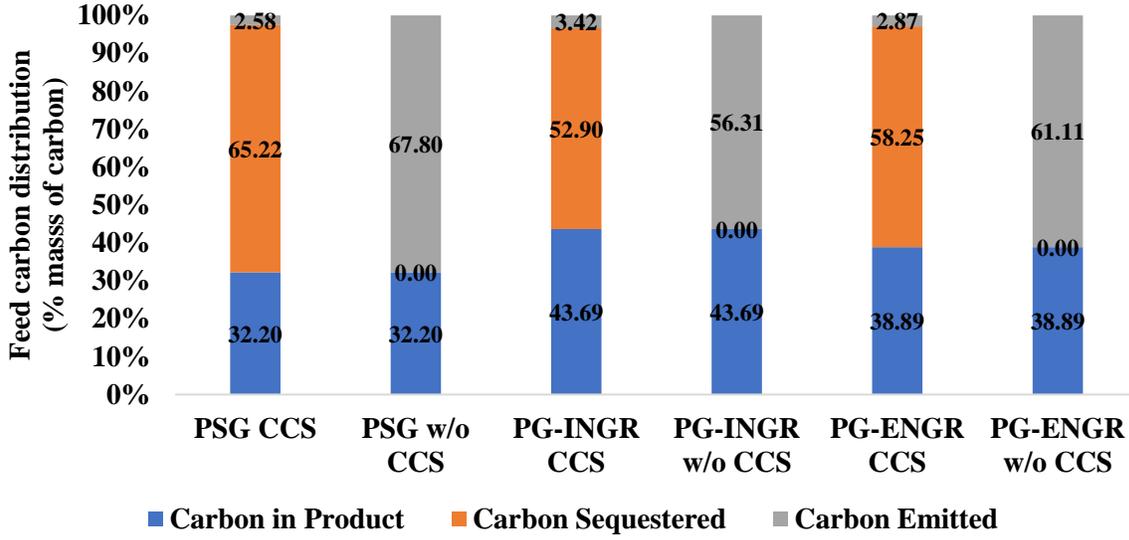


Figure 5: Carbon distribution for each of the design configurations

3.3.2 Fuel and Energy efficiencies

The efficiency of the design to convert the fuel to desirable product is defined as fuel efficiency (η_{fuel}) which is given as:

$$\eta_{fuel} = \frac{Diesel_{HHV} + Gasoline_{HHV}}{Fuel_{HHV}}$$

The efficiency of fuels conversion which takes into consideration all the total energy input to the system is defined as energy efficiency η_{energy} which is given as:

$$\eta_{energy} = \frac{Diesel_{HHV} + Gasoline_{HHV}}{Fuel_{HHV} + Electricity\ consumed + Utilites\ consumed}$$

where $Diesel_{HHV}$, $Gasoline_{HHV}$, and $Fuel_{HHV}$ are the high heating values (HHV) of diesel product, gasoline product, and fuels (petcoke only or petcoke and natural gas) depending on the design employed.

Fig. 6 shows the fuel and energy efficiencies in HHV% for the different configurations with CCS and w/o CCS. It can be seen that for 1 MJ of petcoke, 0.43 MJ of FT fuel is produced for the PSG

design showing a significant amount of energy that could be extracted from petcoke instead of stockpiling it as routinely done in Canada [9, 63]. This would offset the extra amount of crude oil extracted to meet liquid fuels demand since petcoke, the solid waste of crude processing, can be further converted to produce more transportation fuels.

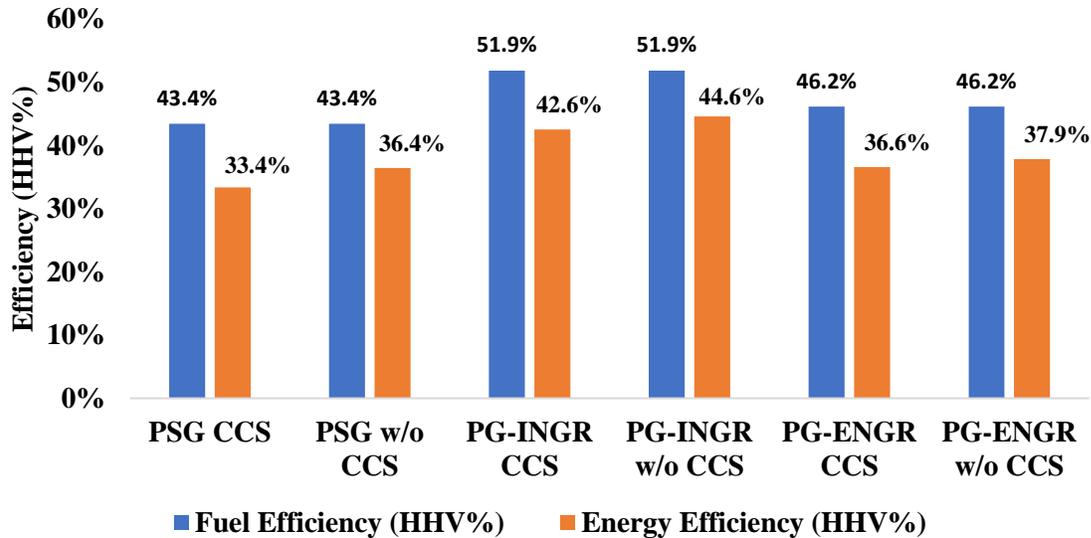


Figure 6: Fuel and energy efficiencies for each of the design configurations

Posing environmental concerns due to the high carbon emissions of the PSG design, this research work explores in a more rigorous fashion other technical and economical viable ways of converting petcoke with minimal environmental impacts. Combining natural gas with petcoke, the fuel efficiency increased to 51.9% and 46.2% for the PG-INGR and PG-ENGR configurations respectively which is of huge significance in fuels production. Energy efficiency for the CCS plants dropped by 10%, 9.3%, and 9.6% points for the PSG, PG-INGR, and PG-ENGR designs respectively showing the extra energy input to the plants. Without CCS, the fuel efficiency remains same but increases for the energy efficiency due to the reduced amount of thermal requirement when the plant operates without CCS. Overall, the PG-INGR configuration with an energy efficiency of approximately 42.6% (with CCS) shows a design that is comparable with commercial petcoke plant [21]; thus, exhibiting a sign of competitiveness.

3.4 Economic analysis

The profitability assessment of the petcoke configuration strategies was carried out and the results summarized in table 8 which shows the detailed cost breakdown of the total capital investment (TCI), operating costs, and product revenues. The results presented in this table are for the petcoke feed capacity of 219 tonnes/day which is consistent with the work of NETL [14].

Table 8: Economic summary for different configurations

Scenario	PSG	PSG	PG-INGR	PG-INGR	PG-ENGR	PG-ENGR
Design Configuration	Yes	No	Yes	No	Yes	No
CCS Enabled	Yes	No	Yes	No	Yes	No
Capital Cost by section(M\$)						
Air Separation Unit	68.6	68.6	70.9	70.9	77.3	77.3
Solid handling	3.1	3.1	3.1	3.1	3.1	3.1
Slurry Prep & Feed	34.2	34.2	34.2	34.2	34.2	34.2
Gasification	180.4	180.4	180.4	180.4	180.4	180.4
Ash/Slag silos	0.3	0.3	0.3	0.3	0.3	0.3
Water Gas Shift	33.7	33.6	34.1	34.1	34.6	34.6
Pre-reformer	-	-	9.1	9.1	9.1	218
Natural gas reformer	-	-	90.2	90.2	44.6	77.4
Acid Gas Removal	169.9	72.2	212.7	86.9	226.8	101.7
CO ₂ Compression	9.4	-	9.3	-	9.7	-
Claus Unit	48.8	48.8	48.6	48.6	51.3	51.3
Pressure Swing Adsorption	11.6	11.6	15.7	15.7	14.6	14.6
Fischer-Tropsch Synthesis	131.3	131.3	208.6	208.6	157.7	157.7
Cooling Tower	13.7	12	10.3	80.0	15.3	10.8
Heat Exchanger Network/Steam system	164.7	139.7	149.4	55.0	207.9	241.1
Cost breakdown at 85% capacity factor						
Total capital investment (M\$)	1116.8	944.8	1382.4	1184.9	1370.0	1162.8
Annual operating cost (M\$/yr)	246.8	371.4	361.5	476.0	335.4	487.8
Total labour cost (M\$/yr)	14.7	14.7	14.7	14.7	14.7	14.7
Total maintenance cost (M\$/yr)	90.0	76.2	111.4	95.5	110.4	93.7
Operating overhead (M\$/yr)	14.2	12.5	16.9	14.9	16.7	14.7
Property insurance & tax (M\$/y)	17.4	14.7	21.5	18.5	21.3	18.1
Petcoke cost (M\$/yr)	0.00	0.00	0.00	0.00	0.00	0.00
Natural gas cost (M\$/yr)	-	-	52.3	52.3	52.3	52.3
Total Utility costs ((M\$/yr)	88.4	48	127	78.7	95.6	70.1
Sulfur sales(M\$/yr)	9.9	9.9	9.9	9.9	9.8	9.8
Gasoline sales (M\$/yr)	97.9	97.9	162.8	162.8	145.0	145.0
Diesel sales (M\$/yr)	268.2	268.2	439.6	439.6	390.9	390.9
Gross earnings (M\$/yr)	375.9	375.9	612.3	612.3	545.7	545.7

Net present value (M\$)	74.3	-588.7	714.2	294.1	489.2	-212.5
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One of the reasons why the PG-INGR and PG-ENGR designs appears much more profitable than the PSG design in table 9 is from economy of scale, since the designs using natural gas use considerably more feedstock. Therefore, the profitability analysis was repeated such that the six designs were scaled to have the same thermal input as the PSG design which is equivalent to a thermal input of 2108 MW (HHV), as summarized in table 10. As a result, these designs all had approximately the same capital cost as well (approximately \$1 billion), and so are suitable for comparison on the basis of similar capital investment.

Table 10: Economic summary for the scaled designs for the 6 different configurations

	PSG	PSG	PG-INGR	PG-INGR	PG-ENGR	PG-ENGR
	Yes	No	Yes	No	Yes	No
Petcoke rate (tonnes/h)	218.7	218.7	159.2	159.2	159.2	159.2
Radiant heat recovered (MW)	216	216	157	157	157	157
Natural Gas rate (tonne/h)	-	-	38.1	38.1	38.1	38.1
Plant Electricity consumed (MW)	232.2	198.4	198.5	174.0	229.2	196.8
Gasoline produced (ML/yr)	232.0	232.0	281.1	281.1	250.4	250.4
Distillate produced (ML/yr)	627.2	627.2	748.3	748.3	665.5	665.5
Sulfur produced (ktonnes/yr)	99.8	99.8	72.5	72.5	72.1	72.1
Direct GHG emitted (MtonnesCO ₂ eq/yr)	0.1	3.6	0.2	2.6	0.1	2.9
Indirect GHG emitted (MtonnesCO ₂ eq/yr)	0.8	0.4	0.7	0.5	0.8	0.7
Total cradle to plant exit gate GHG (kgCO ₂ eq/GJ)	17.7	76.2	13.2	49.3	16.6	62.9
Total capital Cost (M\$)	1116.8	944.8	1140.3	976.6	1129.3	958.2
Annual operating Cost (M\$/yr)	246.8	371.4	282.2	363.2	268.4	372.1
NPV (\$million)	74.3	-588.7	289.2	-3.7	125.3	-412.7
Min. Diesel Selling Price (\$/gal)	1.78	2.32	1.62	1.85	1.74	2.18
Max. Petcoke price (\$/tonne)	6.4	-44.1	35.6	-0.4	15	-44.3
CCA (\$/tonneCO ₂ eq)	379.3	-	175.9	-	301.5	-

When comparing the plants in this way, the combined petcoke and natural gas designs still have higher product yields, higher NPVs, lower GHG emissions per product delivered, and lower CCAs compared to the petcoke only design, showing that integrating natural gas is fundamentally superior in the most important metrics. Furthermore, PG-INGR has 12% more product yield and almost half of the CCA than PG-ENGR, which clearly attests to the improved performance of the

integrated design. However, it was observed that the PSG and PG-ENGR designs are similar in terms of absolute emissions rates and power consumption.

For ease of comparison with current market price, the minimum diesel selling prices for each of the configurations was computed. Even with carbon emission taxes, it can be seen that all the plants with CCS have MDSPs which are competitive with the current refinery diesel wholesale price of \$1.85/gal [52]. Those without CCS are not profitable due to the carbon taxes assumed in this analysis, and hence cannot compete. However, with no carbon taxes on emissions, they turn out to be more profitable given the reduced investment and operating costs. At this scale of operation, the CCAs for the PG-ENGR and PG-INGR designs are \$301/tonne and \$176/tonne respectively, clearly showing the strong effect of economy of scale. Nevertheless, the \$176/tonne CCA for the PG-INGR design is still comparable to or better than other alternative fuels, such as biological biobutanol (\$472/tCO_{2e}) [64], thermochemical biobutanol (\$136/tCO_{2e}) [65], biodiesel (\$400/tCO_{2e}) [66], or corn ethanol (potentially up to \$750/tCO_{2e}) [66].

Another important metric explored was the maximum petcoke price since the valuation of petcoke waste is uncertain. In the previously discussed results, the petcoke price was assumed to be \$0/tonne [14] since it is a locally produced waste. However, the maximum petcoke price was computed as the price at which the NPV becomes zero, with all other parameters at their default values. As shown in Table 10, for all the CCS plants, the maximum petcoke prices were between \$9/tonne to \$44/tonne. For the non-CCS plants, the maximum price was negative, meaning that in order for those plants to be profitable, the processing plant would have to be paid to take waste petcoke off of the hands of the refinery.

3.5 Sensitivity analysis

The economic results presented above are based on investment assumptions and current market prices of commodities which are uncertain and can vary widely due to plethora of reasons such as inflation, demand, politics, etc. Thus, there is a need to carry out a sensitivity analysis. Figure 7 shows the effect of the petcoke purchase price on NPV. Between \$0/tonne to \$50/tonne, the PG-INGR configuration with CCS shows to be the best design and profitable as long as the petcoke price is below \$45/tonne. The PSG and PG-ENGR CCS design are only profitable when petcoke price is no more than \$5/tonne and \$15/tonne respectively. As the petcoke price increased, the PG-ENGR fared better because of the reduced proportion of petcoke it consumes when compared to

the PSG design. Without CCS, none of the plants are profitable (because of the assumed carbon tax).

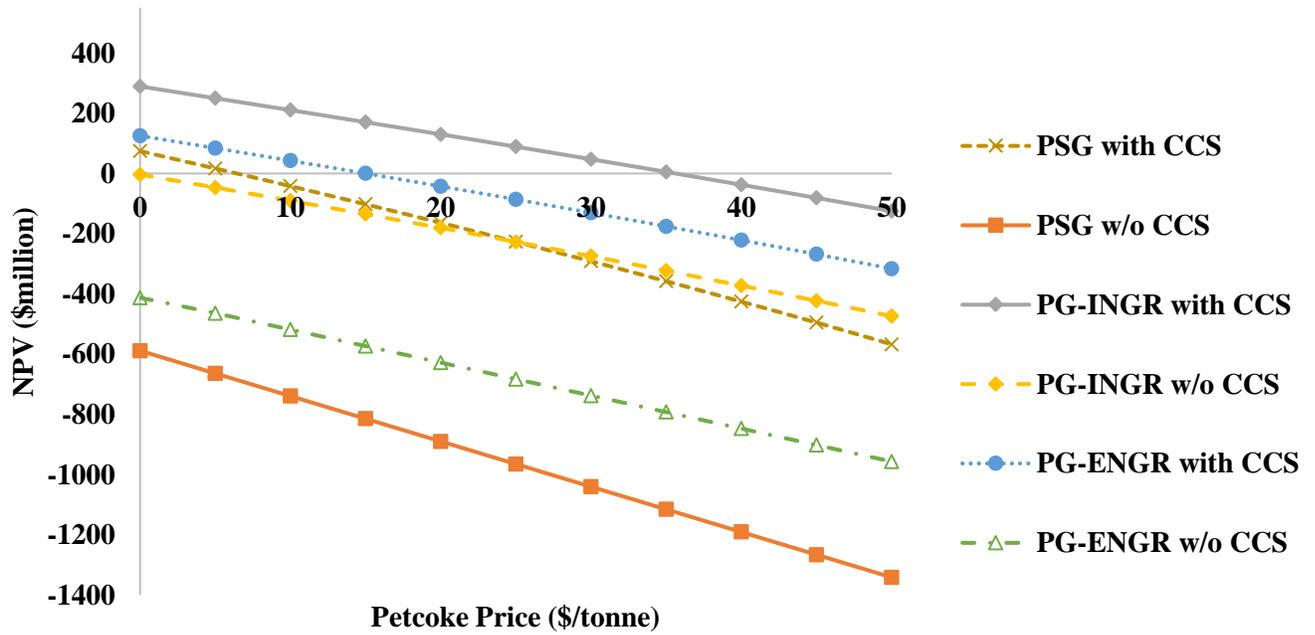


Figure 7: Effect of petcoke price on NPV

The natural gas price is also crucial to the economics of the plant. The range of natural gas prices evaluated is representative of the previous 10 years' price history, and shown in fig. 8. As our utilities were assumed to be a function of the natural gas price, the gas price has significant effect on all the designs, even those that do not use natural gas as a feedstock. Unlike the PGS design with CCS, the PSG design without CCS (less utility consumed) had an increase in NPV when the gas price was increased due to the extra revenue generated from the HPS produced in the gasifier radiant coolers. Compared to the PG-ENGR design which also produces steam in the radiant cooler, the cost of amount of natural gas feed consumed balanced the extra revenue from selling the steam. Despite this condition, the PG-INGR design which uses its heat for syngas generation is still a good investment at a gas price of \$4/MMBtu or below.

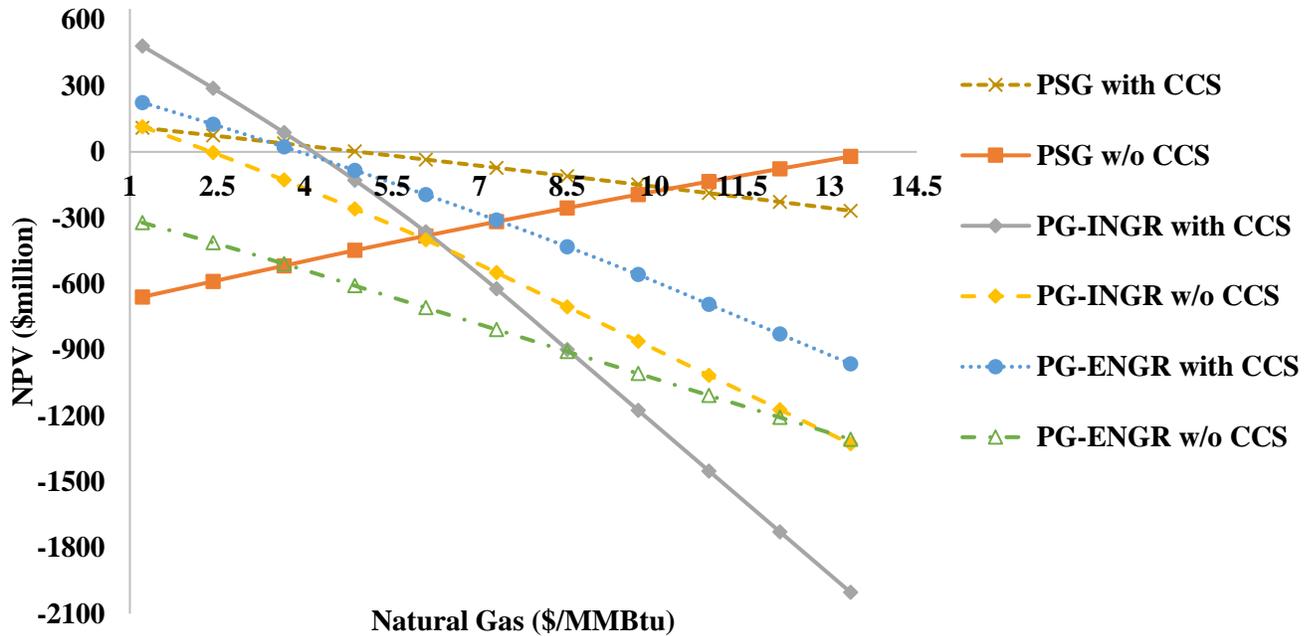


Figure 8: Effect of natural gas price on NPV

The effect of penalizing a plant by the amount of CO₂ emitted was evaluated in fig. 9 and it shows that plants with CCS are almost independent of emissions tax since they have almost no CO₂ emissions. Without CCS, the impact of the CO₂ penalty is well pronounced as can be seen by the huge drop in NPV. The PSG and PG-ENGR designs remain profitable at a tax rate of about \$30/tonne while the PG-INGR could survive till \$49/tonne. One observation is that running the PSG without CCS is more profitable than that of PG-ENGR if the CO₂ tax is within \$20 given the total emissions (per GJ basis) of the design for a cheaper penalty.

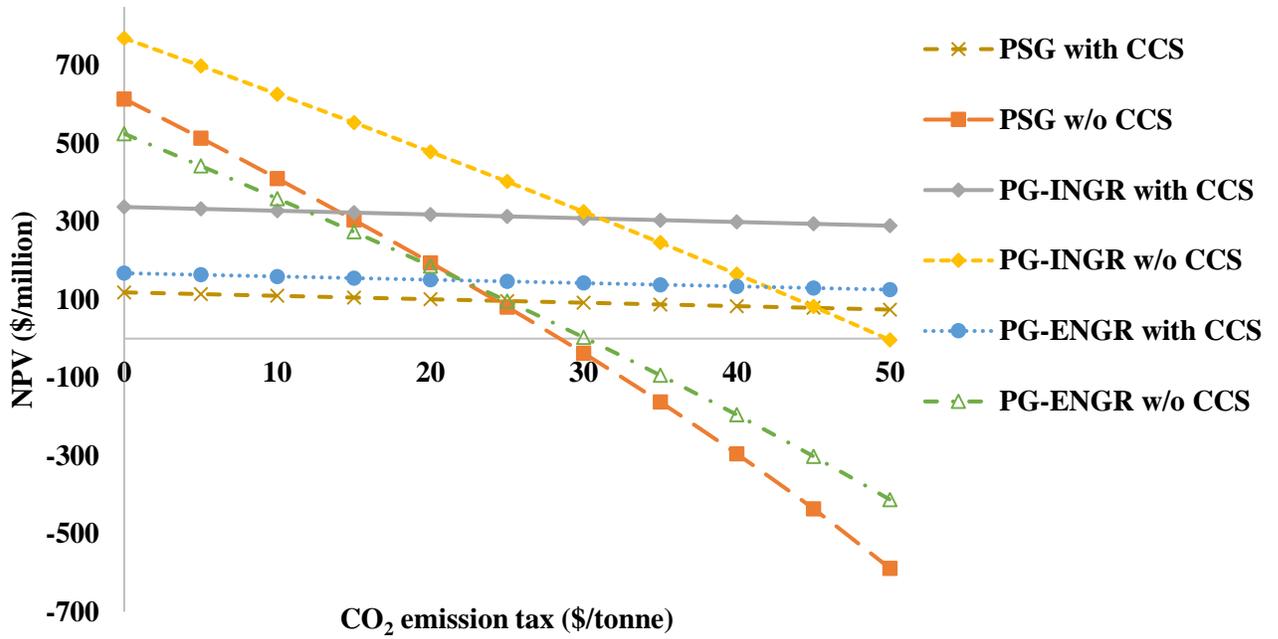


Figure 9: Effect of CO₂ emission tax on NPV

The effects of shareholders interest on the plant is shown in fig. 10. This analysis showed that the CCS plants would have a positive NPV when operated at the recommended D/E ratio of 50:50 [46]. While the PG-INGR design without CCS is profitable at D/E ratio of 81:19, it is not surprising that the PSG and PG-ENGR designs are not profitable even at a D/E ratio of 100/0. Unlike the D/E ratio which had no much impact on the economics of the CCS designs, the effects of IRR (fig. 11) on the NPV showed to be significant.

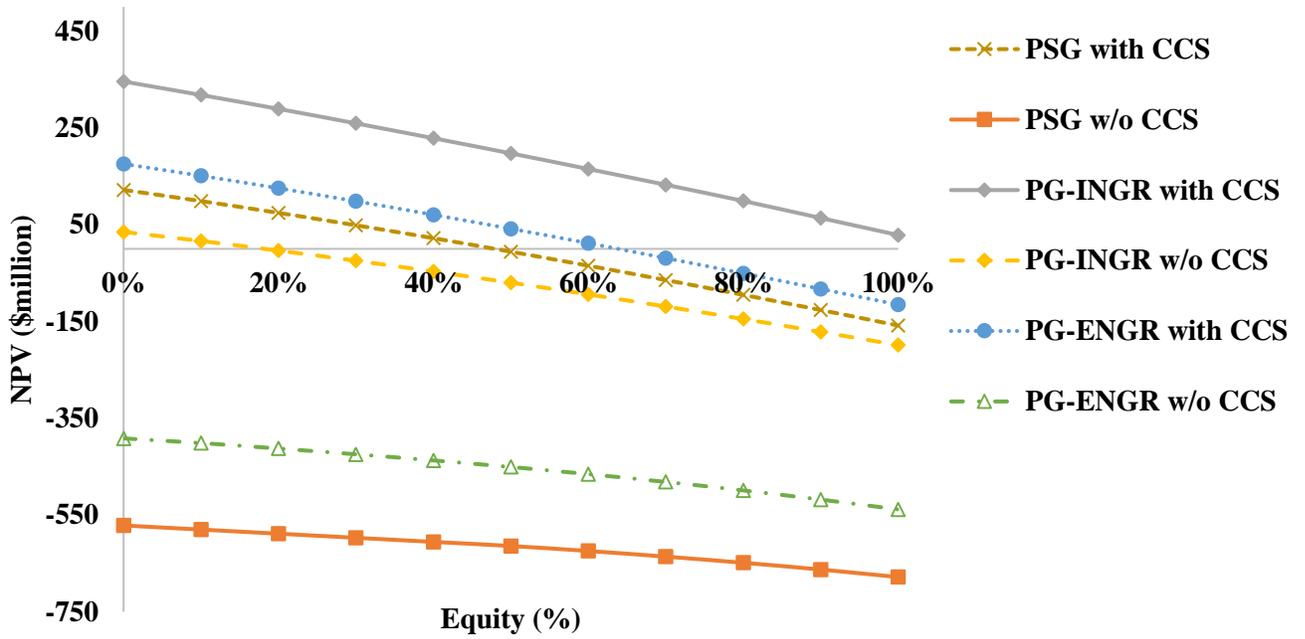


Figure 10: Effect of Equity price on NPV

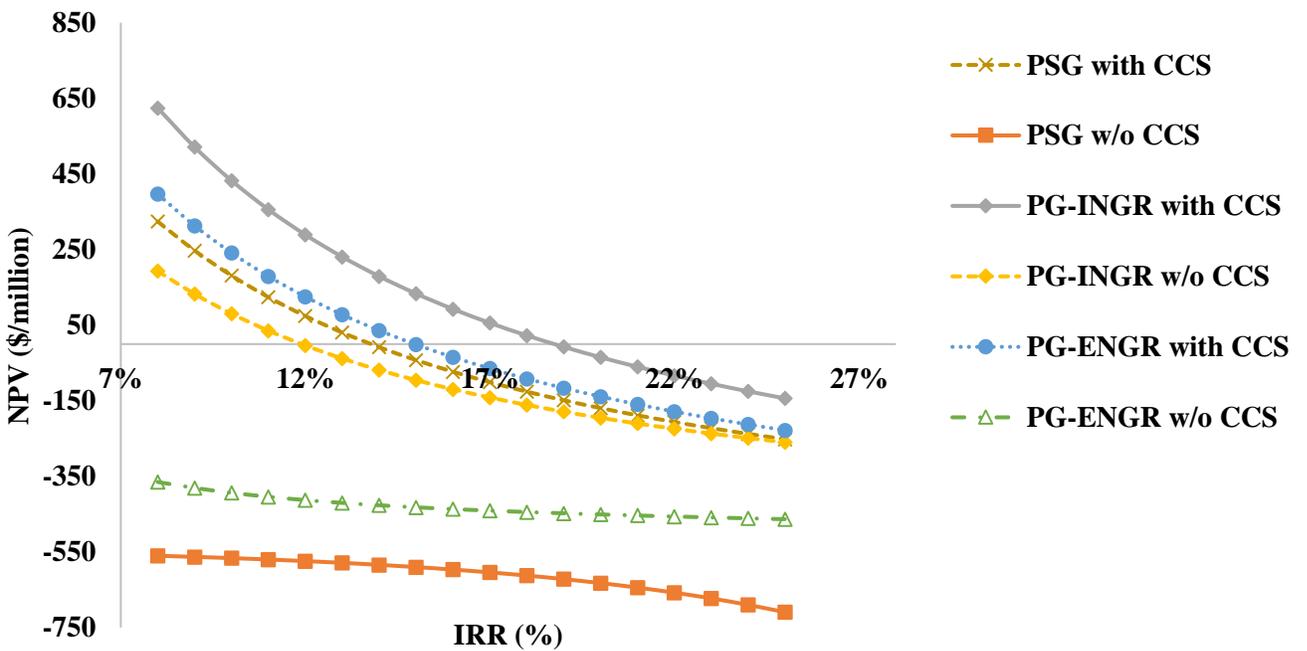


Figure 11: Effect of IRR price on NPV

Interest rates higher than 15% give poor economics for the CCS PG and PG-ENGR designs while the PG-INGR is profitable at up to 18%, which compares well to the recommended IRR of 20% by Worhach et al., [46].

With much uncertainty in the price of crude oil, the price of diesel and gasoline are subject to change. Figures 12 and 13 show the effects of products market price on the profitability of the plant. With only a 4 cents/gal drop in the base price of diesel from our assumed conditions, none of the plants were profitable. Similarly, at a 7 cents/gal drop in gasoline price from the base case was enough to bring the NPV below zero of the most profitable process. So the consideration of this uncertainty would be crucial in future decision making with regards to this process.

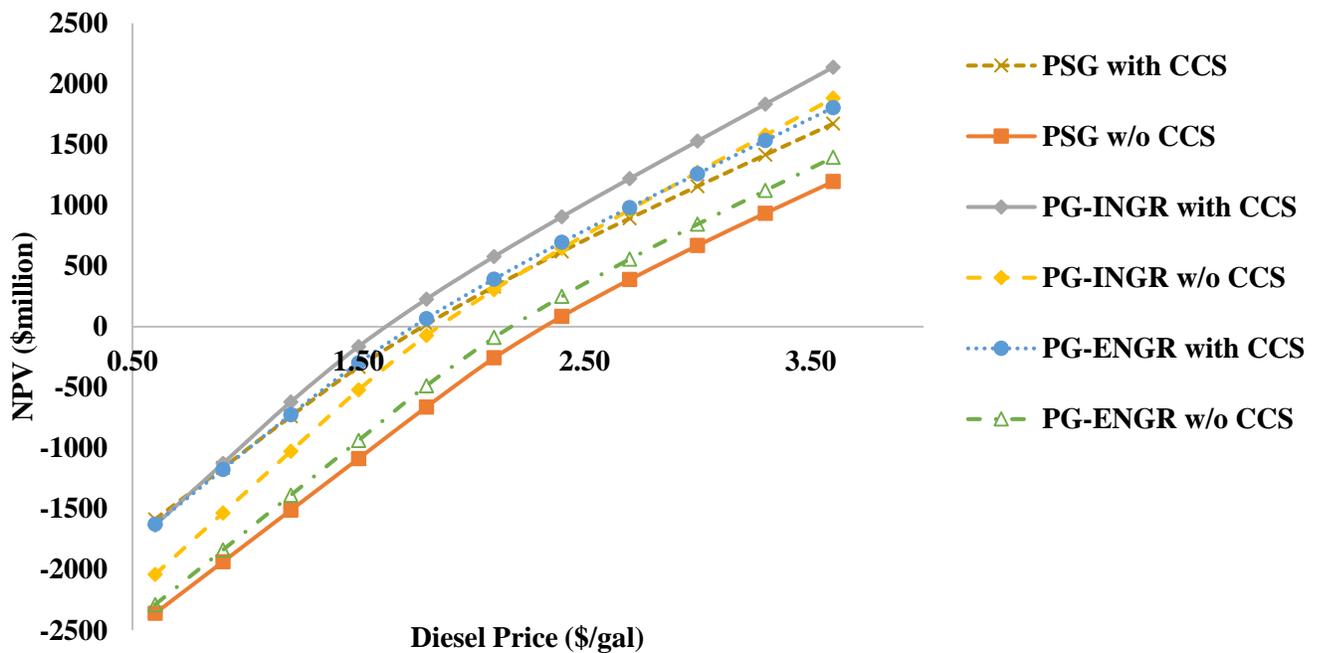


Figure 12: Effect of diesel price on NPV

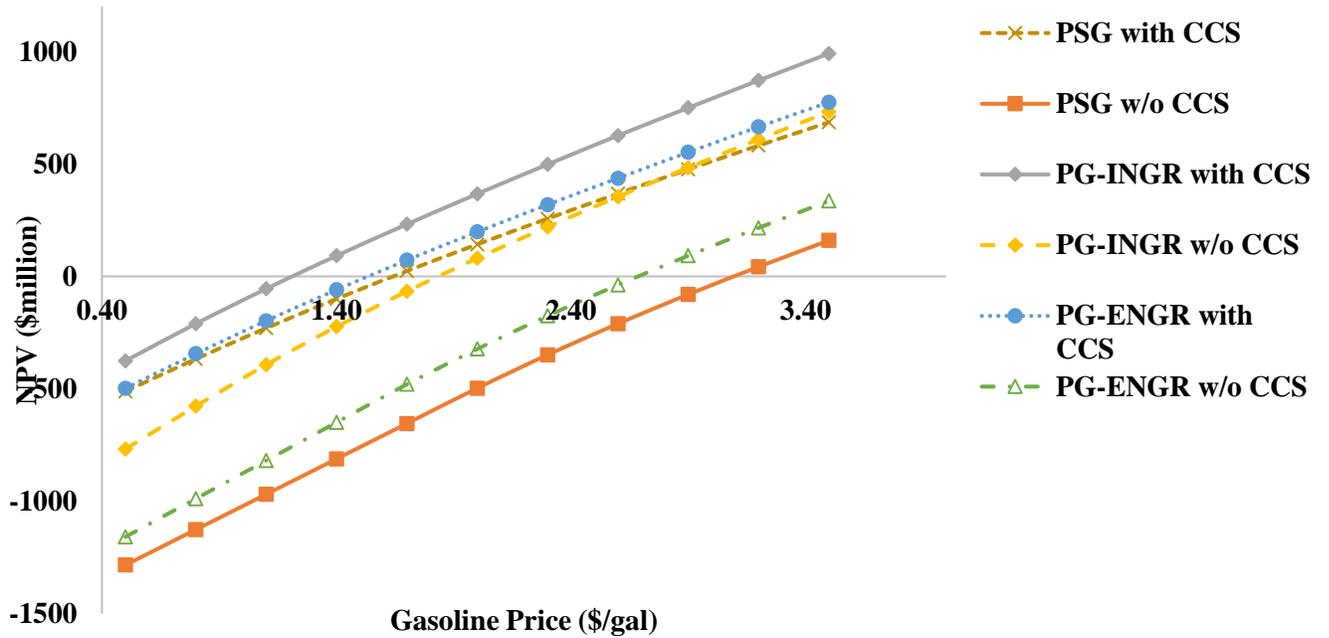


Figure 13: Effect of gasoline price on NPV

To justify the assumption for the cost of the proposed integrated gasifier radiant syngas cooler and natural gas reformer, fig. 14 shows the effect of this assumed cost on NPV. PG-INGR with CCS, the design is profitable even when proposed design is double the cost of a traditional gasifier. The PG-INGR design without CCS has a positive NPV when its cost was less than about 48% more than the cost of a traditional gasifier. Hence, the assumption of a 50% cost is conservative.

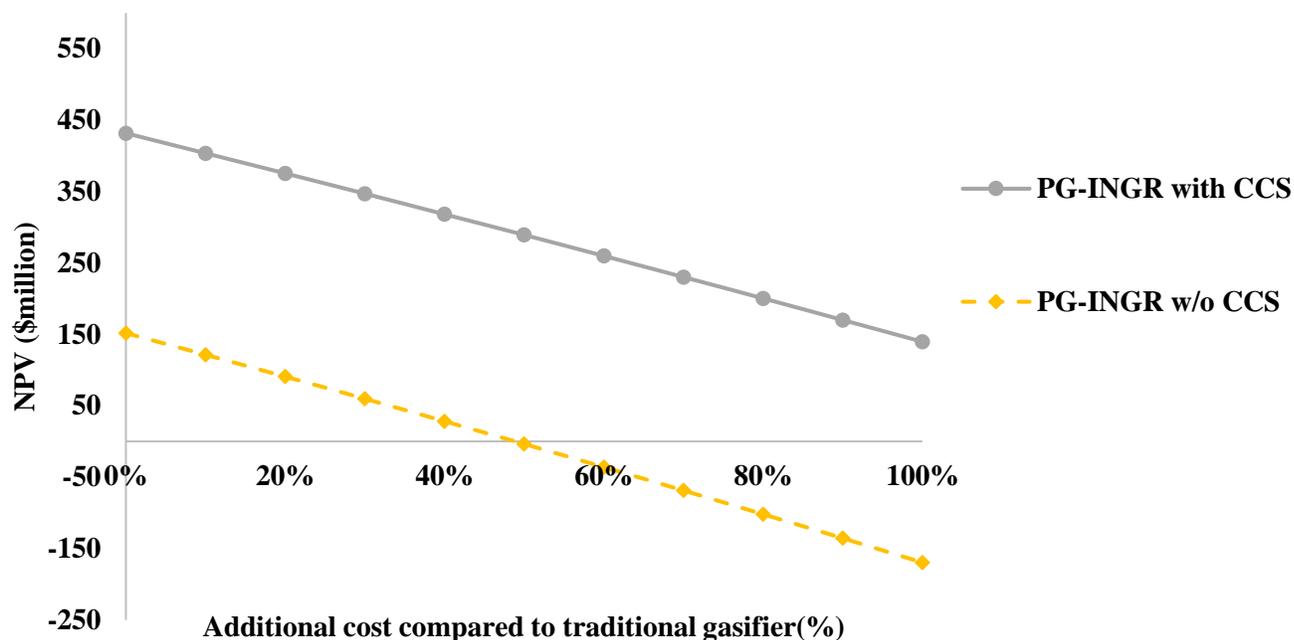


Figure 14: Effect of PG-INGR gasifier cost on NPV

4.0 Conclusions

The results showed that converting petcoke into liquids with CCS through a traditional gasification route is not profitable nor were the environmental benefits worth the cost. However, by tightly integrating natural gas reforming with petcoke gasification (by performing the gas reforming in the tubes of the radiant syngas cooler), the results were much more promising. This integration strategy uses the excess heat from the gasifier to drive the endothermic reforming process of gas reforming, which has synergistic benefits. The two syngas streams can be blended together to produce a syngas with an H₂/CO ratio much closer to the ratio needed for FT synthesis. This avoids some of the losses associated with syngas upgrading (such as water gas shift) or high-temperature heat production (for natural gas reforming). The results showed that this resulted in a substantially more efficient process than an equivalent process using the same amount of petcoke and natural gas, but in a more traditional manner.

This translated into both significant economic and environmental gains such that the PG-INGR process with CCS had a strong business case using the reference market prices. Furthermore, the cradle-to-product GHG emissions were low enough such that there is an incentive to construct the PG-INGR process for the explicit purpose of GHG emissions reduction. For the standard petcoke

consumption rate of 219 t/hr, the cost of CO₂ avoided for PG-INGR was as low as \$90/tCO_{2e} when the process is considered in the context of displacing traditional petroleum fuels. However, the analysis also found that these results are strongly influenced by key parameters such as plant capacity, interest rates, and fuel prices such that even minor changes in some parameters could cause the process to become a poor investment. There is additional room for improvement as well, since the process has not been optimized, nor have the other potential environmental benefits besides GHG emissions reduction been examined. Therefore, the PG-INGR concept is worth further study, but should also be the effects of market uncertainty should be carefully considered.

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Nomenclature

Abbreviations

PSG	petcoke standalone gasification
PG-INGR	petcoke integrated natural gas gasification
PG-ENGR	petcoke external natural gas gasification
CCS	carbon capture and storage
HEN	heat exchanger network
MDEA	methyl di-ethanolamine
FT	Fischer-Tropsch
IRR	internal rate of return
NPV	net present value
CCA	cost of CO ₂ avoided

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